Temperature dependence of local states due to $S = 1/2$ impurities and their correlation in a $S = 1$ Heisenberg chain

Pascal Roos and Seiji Miyashita

Department of Earth and Space Science, Osaka University, Toyonaka, Osaka 560-0043

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Abstract

We study the temperature dependence of the low temperature spin configurations, investigating the magnetization profile of the local states due to the impurities and the two point correlation function centered in one of the impurities. This correlation is found to be weak against temperature effects although the magnetization profile in the triplet state is visible up to higher temperatures. Here we introduce a loop cluster quantum Monte-Carlo method with a fixed magnetization M_z in order to study the correlations in the ground state of a given value of M_z. From the population distribution of magnetization, the very small energy gap between the quasi degenerate states due to the impurities is obtained.

I. INTRODUCTION

Since the Haldane conjecture [1], the peculiar properties of quantum spin systems have been interested in. In particular, properties of integer spin antiferromagnetic quantum spin chain have been studied in detail: theoretically [2,3], numerically [5–9] and experimentally [10–12]. There, important concepts of Valence Bond Solid states (VBS) [3] and hidden order parameter [4,13] have been introduced. Studies involving the impurity (non-magnetic impurities and/or magnetic impurities) on spin chains have been also a current topic [14–18].

As far as we know, only few of them deal with these impurity problem at finite temperatures. Hence, in the present article we will focus on temperature dependence of local states due to $S = 1/2$ impurities and their correlation in a $S = 1$ Heisenberg chain. Here we mainly use the loop cluster quantum Monte-Carlo method (LCQMC). We will be concerned here with the problem of two $S = 1/2$ spins embedded in a $S = 1$ antiferromagnetic Heisenberg periodic chains. While an impurity causes a doublet state [14], two impurities cause a structure with singlet and triplet states similar to the case of the Kennedy triplet in the edge effects [6,8]. This impurity-induced ground state presents a localized structure around the impurities and it has an inhomogeneous order.

In the next section, we give a quick survey of the LCQMC method used to simulate our system. In Sect. III, we obtain the energy gap between quasi degenerate ground state making use of the population distribution of magnetization. In Sect. IV, we investigate magnetization profile of the impurity system. In Sect. V, temperature dependence of the correlation function is investigated and is compared with the magnetization profile. Sect. VI is devoted to the summary and discussion where we also discuss the metastability of local states making use of snapshot obtained in a world-line updating algorithm..

II. MODEL AND METHOD

The model we deal with in this paper is the one dimensional antiferromagnetic Heisenberg $S = 1$ system where we replace some of the spins by $S = 1/2$ impurities. The general hamiltonian of this model is written as

$$\mathcal{H} = J \sum_i \vec{S}_i \vec{S}_{i+1} + J' \sum_{i'} (\vec{S}_{i'-1} \vec{\sigma}_{i'} + \vec{\sigma}_{i'} \vec{S}_{i'+1}), \tag{1}$$

where the first summation concerns the bonds of $S = 1$ spins and the second one the contribution due to the impurities. Here S (resp. σ) represents spin one (resp. one-half). Since we are interested in a purely antiferromagnetic case, J and J' are both positive and we adopt the periodic boundary condition.

In this paper we consider the lattice with two impurities specifically. The impurities are located on sites ensuring a maximum severing compatible with the periodic boundary condition, and the ratio J'/J is fixed to unity. For this particular impurity location, the ground state is expected to be a triplet $S = 1$, with the first exited state of the singlet $S = 0$ just above it, with a small gap Δ_1 between them. This behavior is similar to the edges effects which happen in a pure spin one chain with open boundary conditions. This energy gap corresponds to the gap between the Kennedy triplet and the singlet state in the open chain and is exponentially small with L [6,8]. Thus even at $T = 0.01J$, $\Delta_1 \ll T$ for long chains such as $L = 64$. There is also another gap between the ground state and the excitation continuum, which we will refer as the Haldane gap Δ_H henceforth: $\Delta_H \simeq 0.4J$ in the pure $S = 1$ model. The expected low energy spectrum is presented in Fig. 1. If we shift one of the impurities by one site, the singlet state becomes the ground state and the triplet states locate above it, although the global excitation spectrum is similar to Fig. 1.

In order to obtain the finite temperature properties we mainly use the Loop Cluster Quantum Monte-Carlo (LCQMC) method [19]. The LCQMC allows to perform the continuous time calculation easily where we can avoid the Trotter number extrapolation in the traditional World-line Quantum Monte-Carlo (WLQMC) method. The configuration update is done in the LCQMC without conserving the total magnetization or the winding number, on the contrary to the WLQMC. In general, LCQMC releases us from strong autocorrelation and thus allow us to reach to the equilibrium state at very low temperatures. We compared the simulation of LCQMC and a traditional WLQMC. We found that about 10^5 MCS gives good results in the present study by LCQMC, while more than 10^6 are necessary to obtain the results with the same accuracy by WLQMC at $T = 0.1J$.

However, in a simple minded LCQMC we can not specify the value of the magnetization M_z and if some states are nearly degenerate around the ground state, LCQMC always equilibrates among these states. Thus, it is difficult to obtain the true ground state configurations. In WLQMC we can control the value of M_z in the initial state and keep it by suppressing the global flip which changes the magnetization.

This nearly degenerate ground state happens in the present study. Thus it is preferable to control M_z in LCQMC. In this circumstance we introduced a method where we can specify the value of M_z (M_z-specifying LCQMC) in order to avoid this difficulty. There are two ways to control M_z in LCQMC. One is the way where we stop the flip of the clusters of nonzero magnetization. Thus the magnetization in the initial state is kept. The other is the way where we perform standard LCQMC and store the data separately according to M_z. If we need the information for a specific value of M_z, we use the data with that value of M_z only.

Here, we adopted the latter method. In order to check the method we compare the low temperature results obtained by the LCQMC and those obtained by Exact Diagonalization (ED). Since ED is restricted to rather short chains, we compared the result for a chain length of $L = 12$.

In $L = 12$ the gap Δ_1 is rather big due to finite size effects and is about $0.6174J$. Thus, we can study the ground state at $T \ll \Delta_1$. For example $T = 0.01J$ is quite low enough. First we compare data within $M_z = 1$ obtained by ED and the data obtained by the above mentioned method.

We show the profile of magnetization:

$$\{M^z(i)\} = \{\langle\sigma_i\rangle \text{or } \langle S_i\rangle\} \tag{2}$$

for $L = 12$ with $M_z = 1$ obtained by the both methods in Fig. 2. Here we find that the method works very well.

Next, we compare data without specifying magnetization, where we need to sum up the data obtained by ED of the ground states for $M_z = -1$, 0 and 1 in order to compare the data . If we do not specify the magnetization, trivially we have $M^z(i) = 0$. Thus here we compare the correlation function:

$$\{C_j = \langle\sigma_i S_j\rangle\}, \tag{3}$$

where we observe the correlation between a $S = 1/2$ spin σ_i and other spins. In Fig. 3(a) we show the data without specification of M_z obtained by ED and LCQMC, respectively. Here

we again find that the method works very well. We also compare data of the correlation function within $M_z = 1$ in Fig. 3(b). Thus we conclude the method to specify the value of M_z is valid and works practically.

III. ENERGY GAP OF THE NEARLY DEGENERATE GROUND STATES

We can utilize the fact that the equilibrium among nearly degenerate states is rather easily realized in LCQMC, which is difficult in WLQMC. In the equilibrium state, the probability of the triplet state and the probability of the singlet state in the quasi degenerate states are given,

$$p_{\rm t} = {\rm e}^{-\frac{E_G}{k_{\rm B}T}}/Z \quad \text{and} \quad p_{\rm s} = {\rm e}^{-\frac{E_G+\Delta_1}{k_{\rm B}T}}/Z, \tag{4}$$

respectively. Here Z is the partition function. Because the energies of other states are much higher, i.e. the Haldane gap $\Delta_{\rm H}$ is much larger than the temperature: $\Delta_{\rm H} \gg T \gg \Delta_1$, we have

$$p_{\rm t} = \frac{1}{3+{\rm e}^{-\frac{\Delta_1}{k_{\rm B}T}}} \quad \text{and} \quad p_{\rm s} = \frac{{\rm e}^{-\frac{\Delta_1}{k_{\rm B}T}}}{3+{\rm e}^{-\frac{\Delta_1}{k_{\rm B}T}}}. \tag{5}$$

Thus by counting the number of the Monte Carlo steps (MCS) for $M_z = -1, 0$ and 1, say N_{-1}, N_0 and N_1, respectively, we can estimate the Δ_1 from the relation:

$$r = \frac{N_{-1}+N_1-N_0}{N_{-1}+N_1+N_0} = \frac{1-{\rm e}^{-\frac{\Delta_1}{k_{\rm B}T}}}{3+{\rm e}^{-\frac{\Delta_1}{k_{\rm B}T}}}. \tag{6}$$

In Fig. 4 we show the histograms of $\{N_M(T)\}$ for $T = 0.01J$ and $T = 0.2J$. At $T = 0.01J$ we find only $M_z = \pm 1$ and 0 which come from the nearly degenerate four states. On the other hand at $T = 0.2J$ the magnetization distributes up to higher values. In table I we show the value of $\{N_{M_z}\}$ for different temperatures. In order to obtain the gap, in Fig. 5 we plot the gap Δ_1 obtained by

$$-\ln\left(\frac{1-3r}{3+r}\right) = \frac{\Delta_1}{k_{\rm B}T} \tag{7}$$

as function of $k_{\rm B}T$. Here we estimate $\Delta_1 \simeq 0.0047J \pm 0.0002$. Here the error bar is obtained as the standard deviation in the values of Δ_1 estimated at temperatures $T \leq 0.03J$. Although it has been so far difficult to obtain this gap because of the smallness, now we have a method to estimate it, which is one of the advantages of the LCQMC.

IV. MAGNETIZATION PROFILE

Because a doping with S=1/2 causes the local states with rather widely spreaded impurity-induced magnetization, it is expected that the local states of doped spins correlate each other and cause a quasi-long range order in the system. In order to see this correlation of local states, we investigate the magnetization profile in the ground state. By LCQMC, we obtain the profile at $T = 0.01J$. In Fig. 6 we show the magnetization profile for $L = 64$ with $M_z = 1$. Here, the impurities are located on the site 16 and 48. This figure implies the presence of impurity induced Long Range Order (LRO). It is a ferromagnetic LRO of the effective spins of the local states while it is an inhomogeneous antiferromagnetic order of the original spins.

If we study the magnetization profile in the subspace of $M_z = 1$, the local structure should remain till a rather high temperature because of the gap in this subspace is about Δ_H. At high temperatures the correlation between them collapses. In order to see the degree of this correlation, we observe the staggered magnetization:

$$M_{\rm SG} = \sum_{i=1}^{L} (-1)^i S_i^z. \tag{8}$$

In Fig. 7, the temperature dependence of $\langle M_{\rm SG} \rangle$ is shown. Here, we find that the correlation persists until $T_1 \simeq 0.4J$. Even above this temperature we find the local structure remains, but the magnetization of the local state fluctuates in time and thus $\langle M_{\rm SG} \rangle$ vanishes. The local structure persists until $T_2 \simeq 1J$.

In order to investigate the true equilibrium state we have to study the system without specifying the value of M_z. However, if we do not fix the magnetization we do not find any

significant profile, that is $< S_i >= 0$ in principle because of the degeneracy of $M_z = \pm 1$ and $M_z = 0$, even if there exists some steady magnetization profile in each of them. Thus we should investigate the spin correlation function instead of the magnetization profile in order to study whether an intrinsic correlation exists or not.

V. CORRELATION FUNCTION

As pointed out in the previous section, the LRO in the ground state can be viewed as the correlation between the local states. In order to explore the correlation behavior, notably the temperature dependence, we investigate the spatial profile of the two point correlation function $< S_i S_j >$.

Some results for $L = 12$ has been shown in Sect. II. In this section we study a system of $L = 64$. In Fig. 8(a), the correlation function in the $M_z = 1$ subspace at $T = 0.01J$ is shown which represents the ground state configuration. It should be noted that the correlation appears in rather small amount in comparison with the magnetization profile, which can be explained by the trivial relation $| < S_i S_j > | \geq | < S_i >< S_j > |$.

The correlation function without specifying M_z value is presented in Fig. 8(b). Although the local structure around the impurity remains, the correlation function between the two local structures is much reduced. This reduction can be understood from the argument in Sect. III. In the true ground state there are two parallel and one anti-parallel configurations of the local structure. Thus we expects that the correlation between the local states, which corresponds to the values around $i = 48$, is one third of that in Fig. 8(a). However the temperature is higher than the gap Δ_1, and thus the singlet (excited) state also contributes to the correlation. Thus as we discussed in Sect. III, value of the correlation function, C, is estimated as

$$C = (\frac{1 - e^{\frac{-\Delta_1}{k_B T}}}{3 + e^{\frac{-\Delta_1}{k_B T}}}) C_0, \tag{9}$$

where C_0 is the corresponding value in Fig. 8(a). The reduction ratio $(1 - e^{-\Delta_1/k_B T})/(3 + e^{-\Delta_1/k_B T})$ has been estimated in the Sect. III to be 0.105. In Fig. 8(b) at $T = 0.01J$ the

ratio is found to be consistent and we still find some correlation. If the temperature increases up to $T = 0.05J$, the reduction rate is 0.017 and the correlation can not be seen any more. (Fig. 8(c))

On the other hand if we fix the magnetization in $M_z = 1$ the correlation is only gradually reduced as the temperature increases. In Fig. 9(a) we show the temperature dependence of this case. In Fig. 9(b) the summation of the staggered correlation

$$C_{\rm SG} = \sum_{i=1}^{L} (-1)^{|i-j|} S_i^z S_j^z. \tag{10}$$

is shown. Here $C_{\rm SG}$ reduces to half around $T = 0.5J$ which corresponds to T_1 where the correlation between the local state vanishes. The correlation within a local state remains, which results nonzero value of $C_{\rm SG}$ above T_1. $C_{\rm SG}$ begins to grow significantly around $T = 1J$ which corresponds to T_2 in Sect. II where the local state is formed.

VI. SUMMARY AND DISCUSSION

We have investigated the correlation between the impurity induced local magnetic states in $S = 1$ antiferromagnetic chain. By investigating the equilibrium distribution of M_z at very low temperatures, which becomes possible in LCQMC, we find a new method to estimate the energy gap between nearly degenerate states. We have studied how the impurity-induced correlation function, that is to say, the correlation between the local states around the impurities, decays when the temperature increases. We found that the correlation is very weak against the temperature although it is robust in the ground state. The correlation survives only below the temperature of the order of Δ_1 which is the gap between the quasi-degenerate ground state due to the impurity.

Finally we would like to point out the metastable nature of the local state. Because the local state is rather tightly bounded, it tends to move collectively. Thus we expect that the dynamics of the total motion of the cluster is rather slow. If we study the spin configuration in WLQMC we can find rather stable magnetization profile even at high temperatures and

also in $M_z = 0$ subspace, which should be a short time metastable state. In Fig. 10 we show an example of such configuration. In LCQMC the update is very rapid and we can not see such metastable state. If we are interested in the relaxation phenomena after changing parameters of the system, such as switching off the magnetization, etc., the dynamics of such metastable states becomes important. While at high temperatures they relax by the temperature effect, they would relax through quantum tunneling at low temperatures. The quantum mechanical life time of the metastability can be estimated by the correlation length through the Trotter axis, as has been investigated as the local susceptibility in the studies of quantum Griffiths-McCoy singularity [20,21]. Such dynamics will be studied in the future.

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FIGURES

FIG. 1. Schematic low energy spectrum

FIG. 2. Magnetization profile in $M_z = 1$ for ED (circle) and LCQMC at $T = 0.01J$(square)

FIG. 3. Two point correlation function profile for ED (circle) and LCQMC at $T = 0.01J$ (square) (a) without fixing M_z (b) in $M_z = 1$ subspace

FIG. 4. Distribution of M_z for 10^5 MCS (a)$T = 0.01J$ (b)$T = 0.2J$

FIG. 5. Gap Δ_1 estimated at various temperatures by Eq.(7)

FIG. 6. Magnetization profile in $M_z = 1$ at $T = 0.01J$

FIG. 7. Staggered magnetization, Eq.(8), versus T in $M_z = 1$

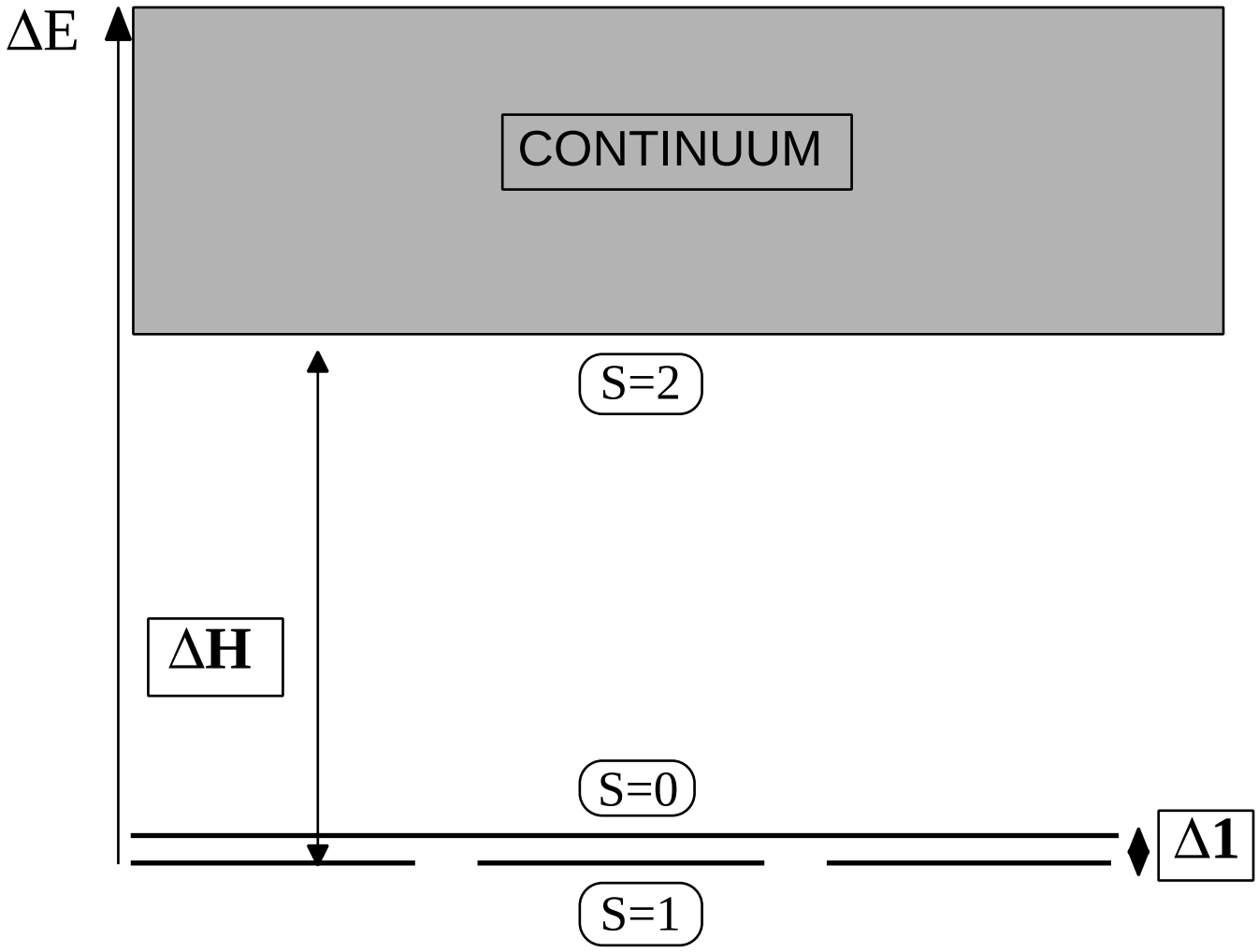
FIG. 8. Two point correlation function profile a) in $M_z = 1$ at $T = 0.01J$ b) without fixing M_z at $T = 0.01J$ c) without fixing M_z at $T = 0.05J$

FIG. 9. a) Two point correlation function for various temperatures within $M_z = 1$ and b) summation of the staggered two point correlation function

FIG. 10. Magnetization profile in a short time for $M_z = 0$ at $T = 0.05J$ obtained by WLQMC which is expected to be a metastable configuration

TABLES

TABLE I. Distribution of $\{N_{M_z}\}$ for various T after 10^5 Monte-Carlo steps



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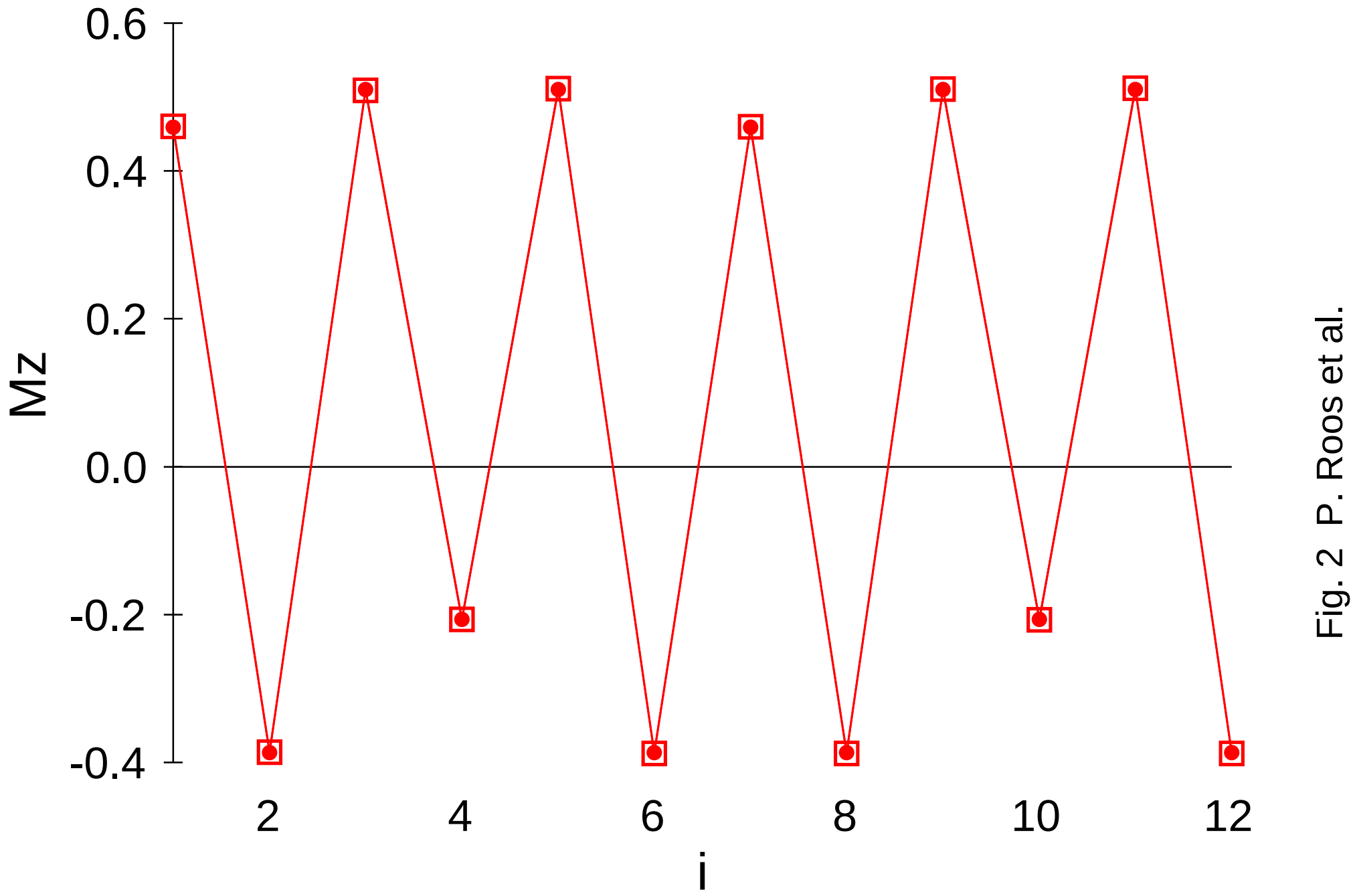

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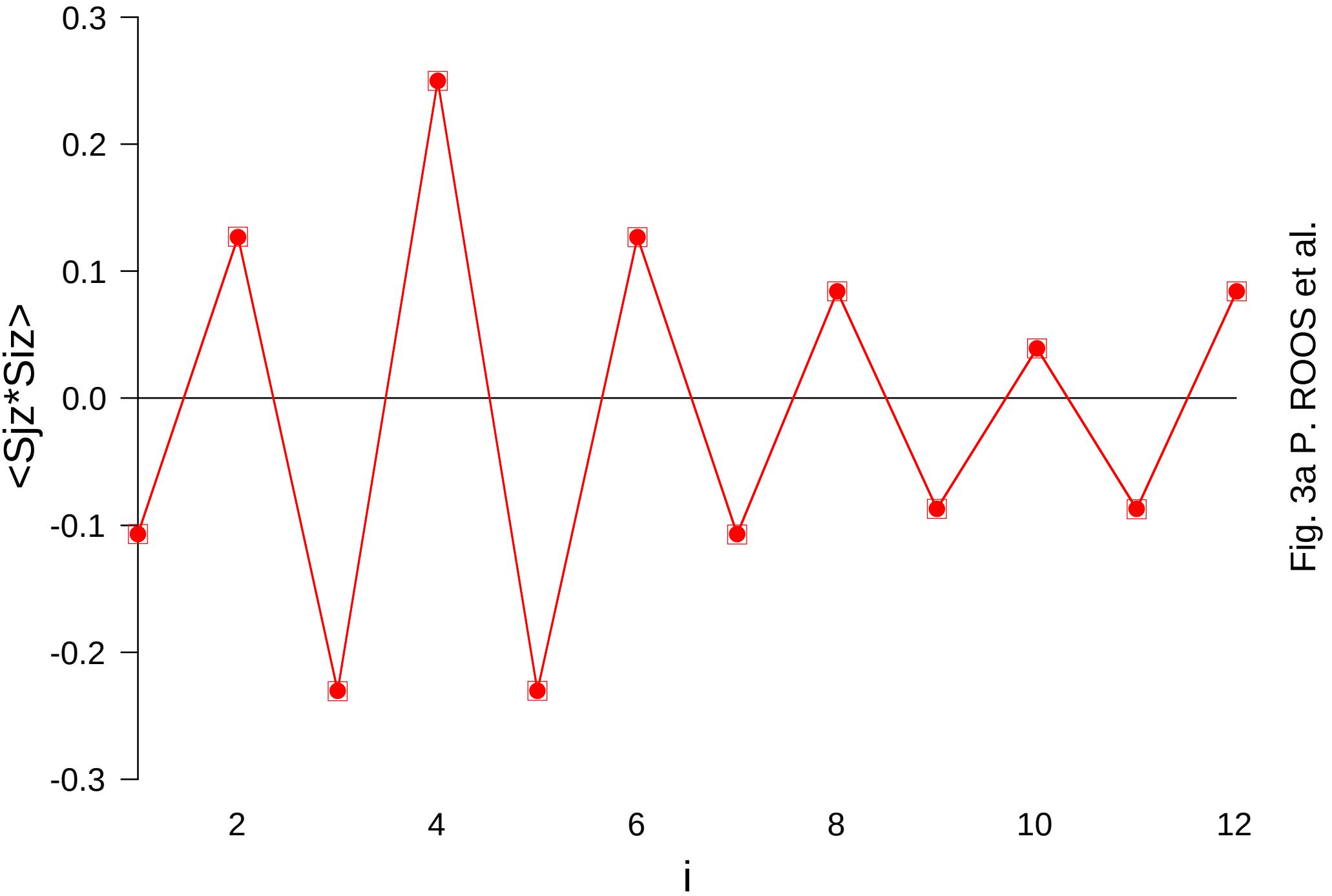
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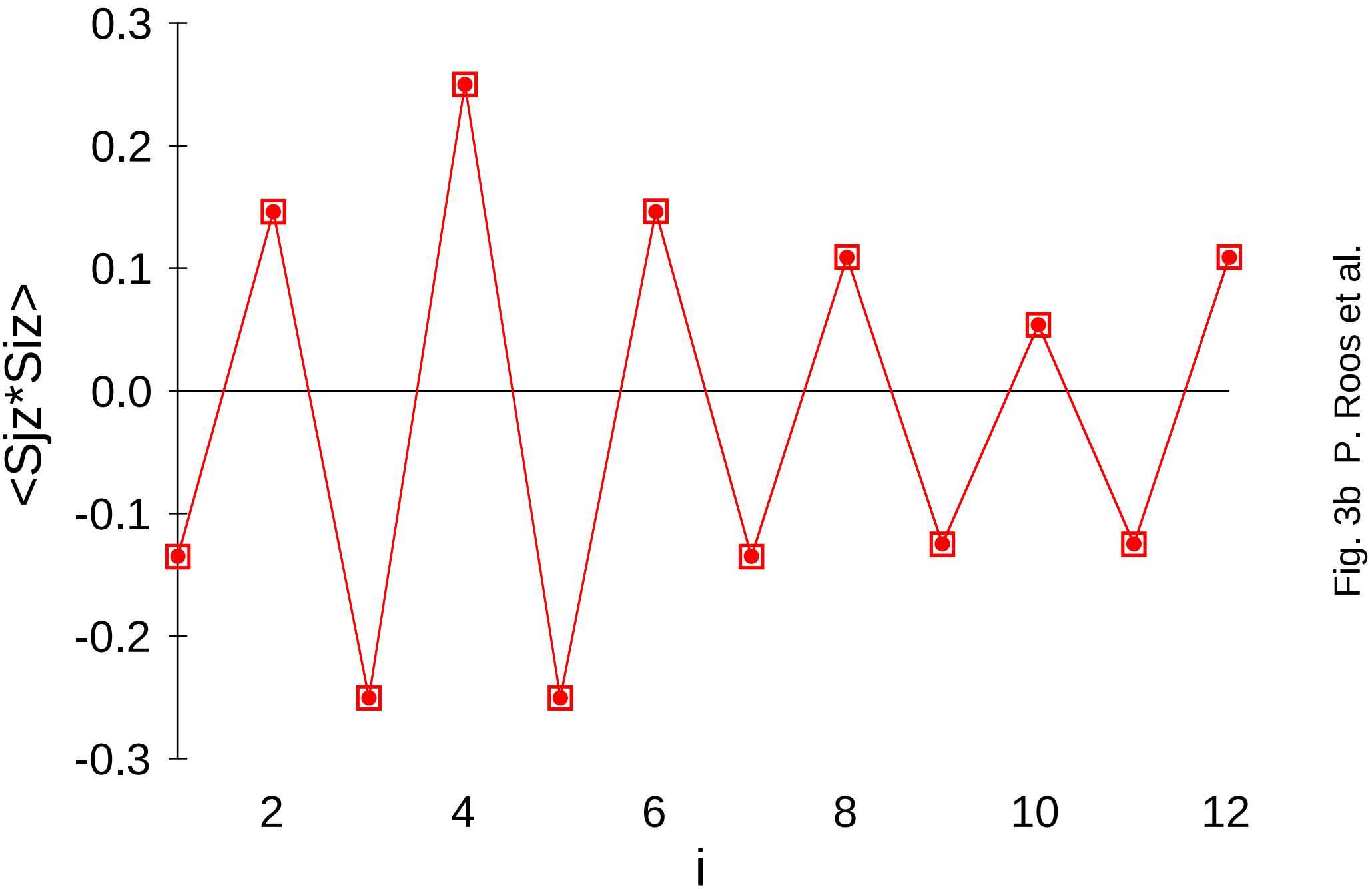
Fig. 3a P. ROOS et al.



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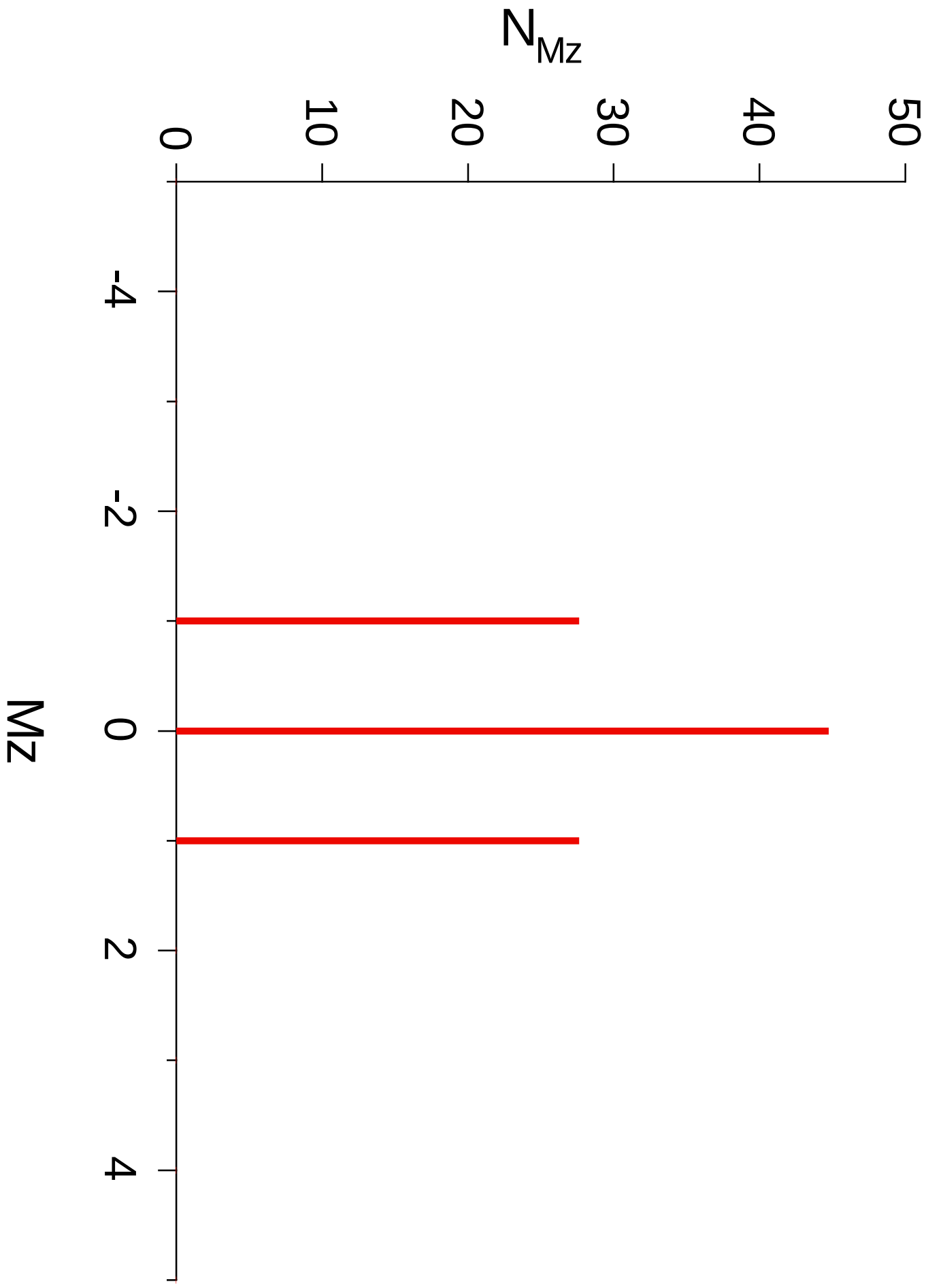

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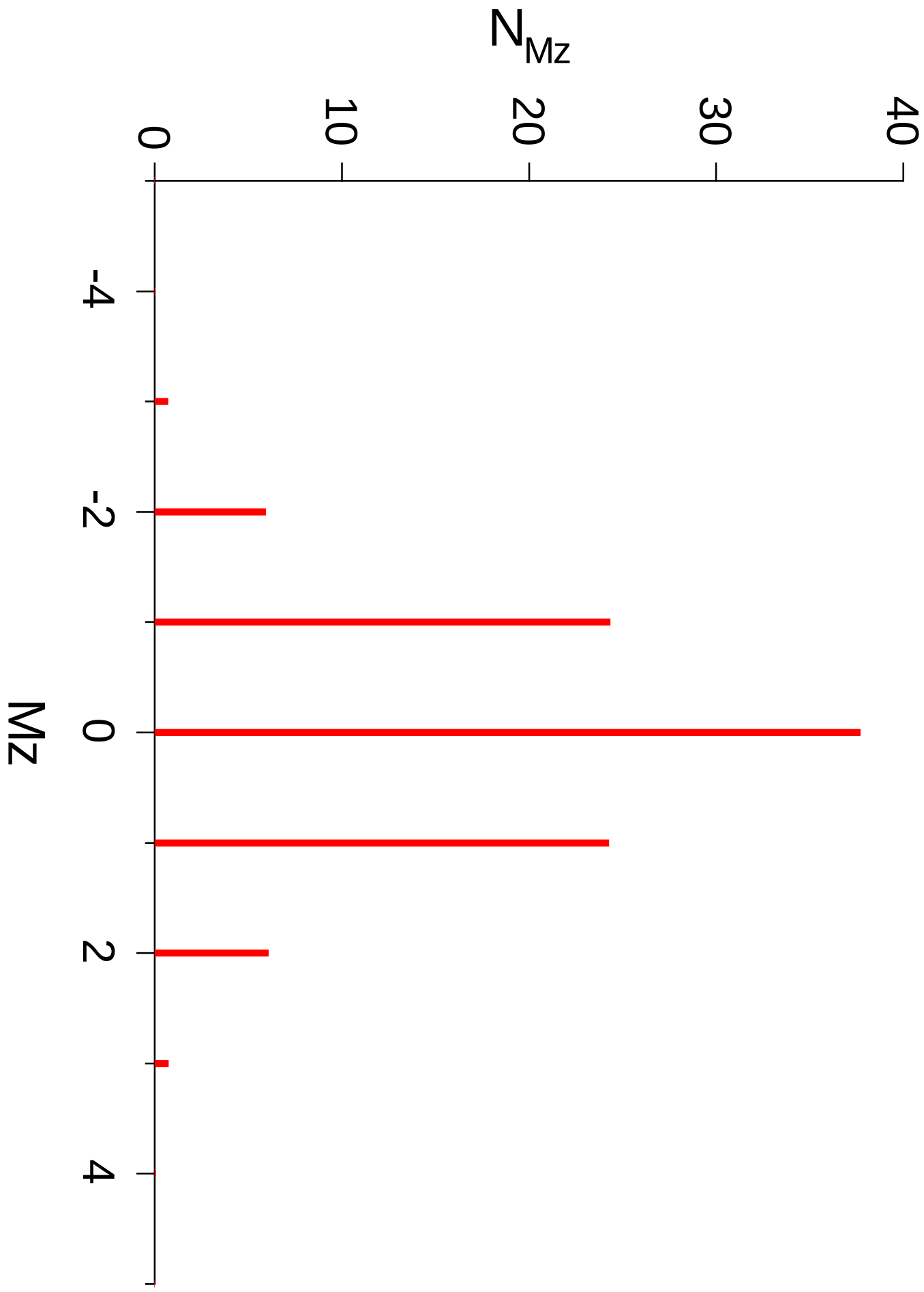

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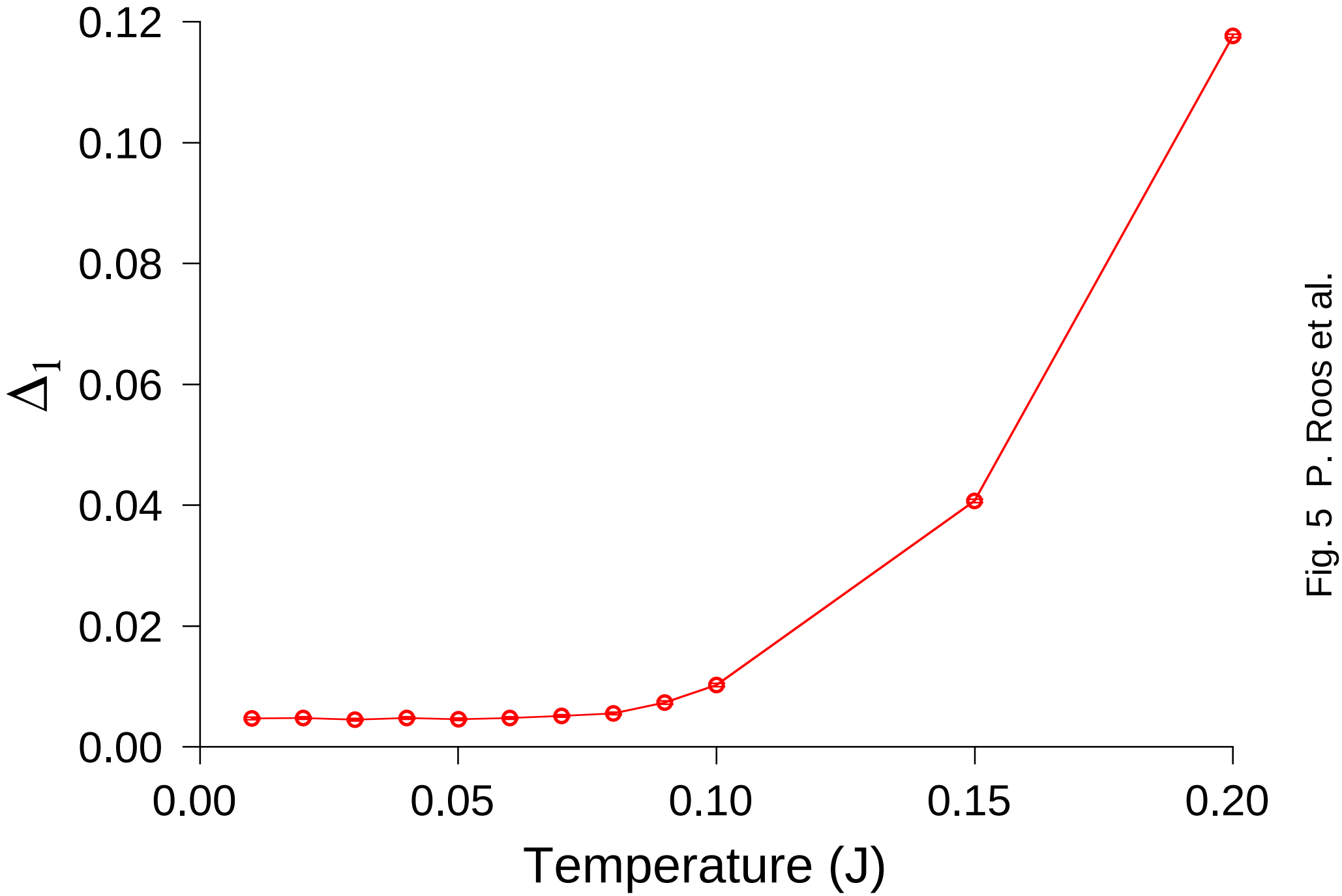

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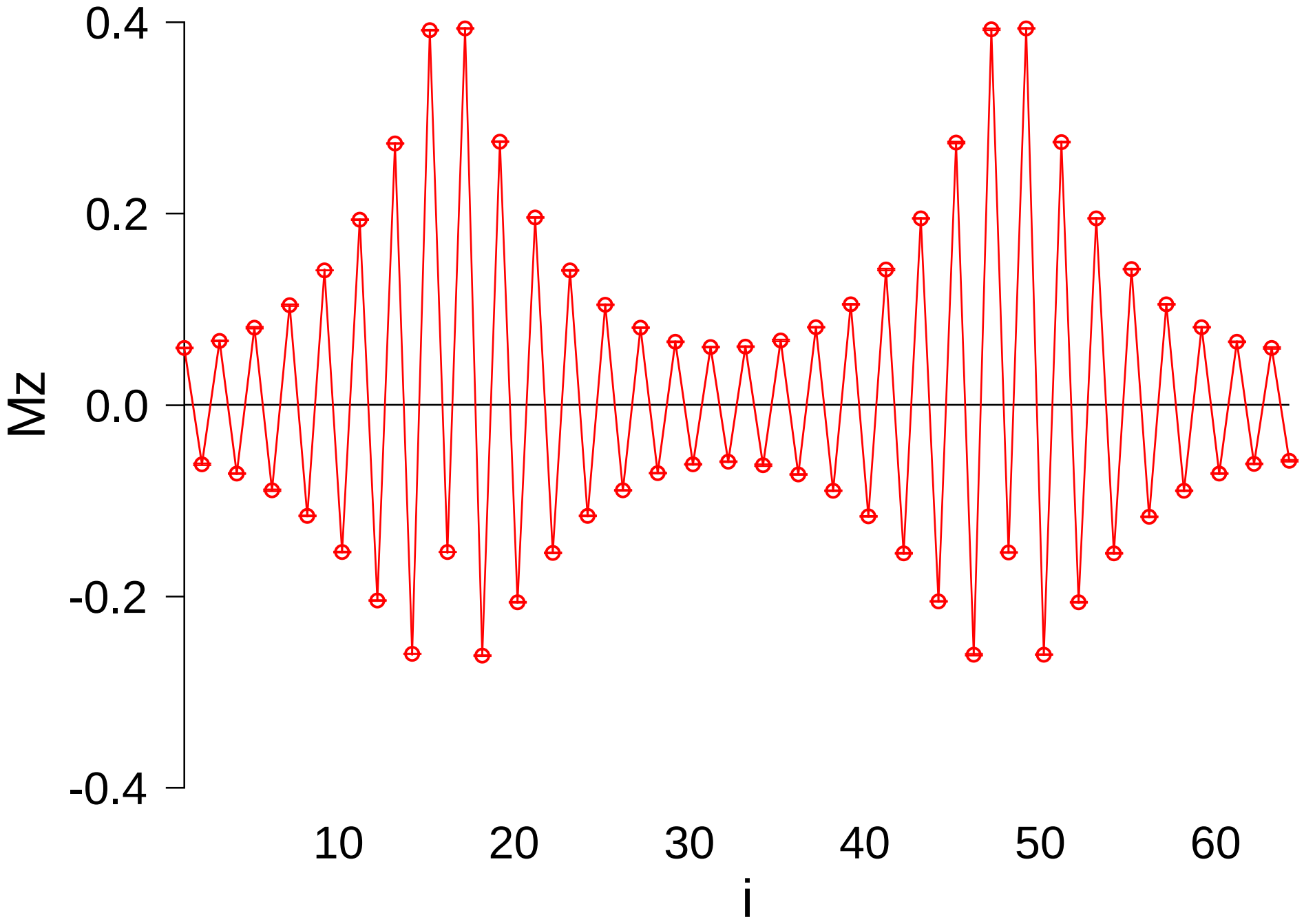

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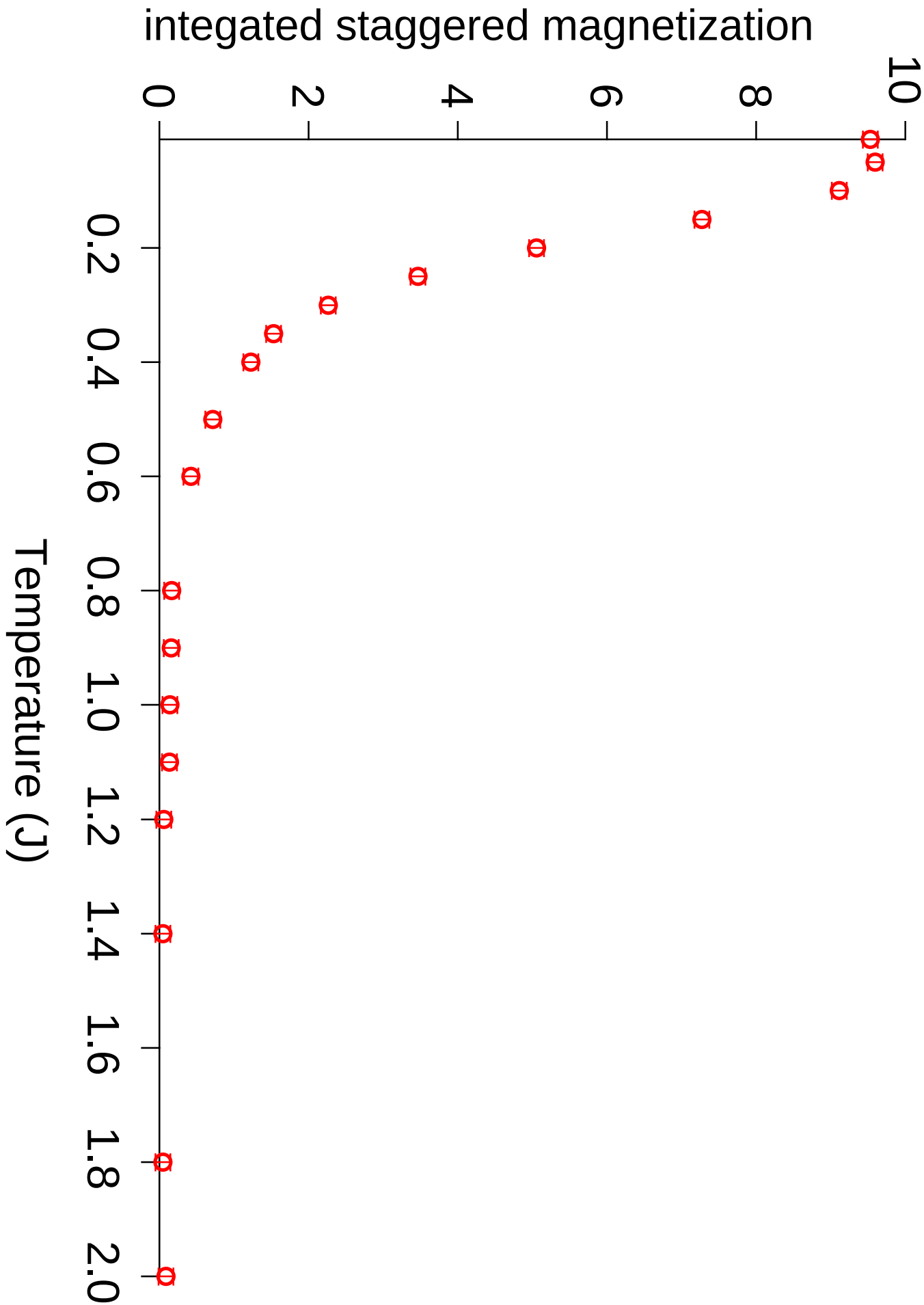

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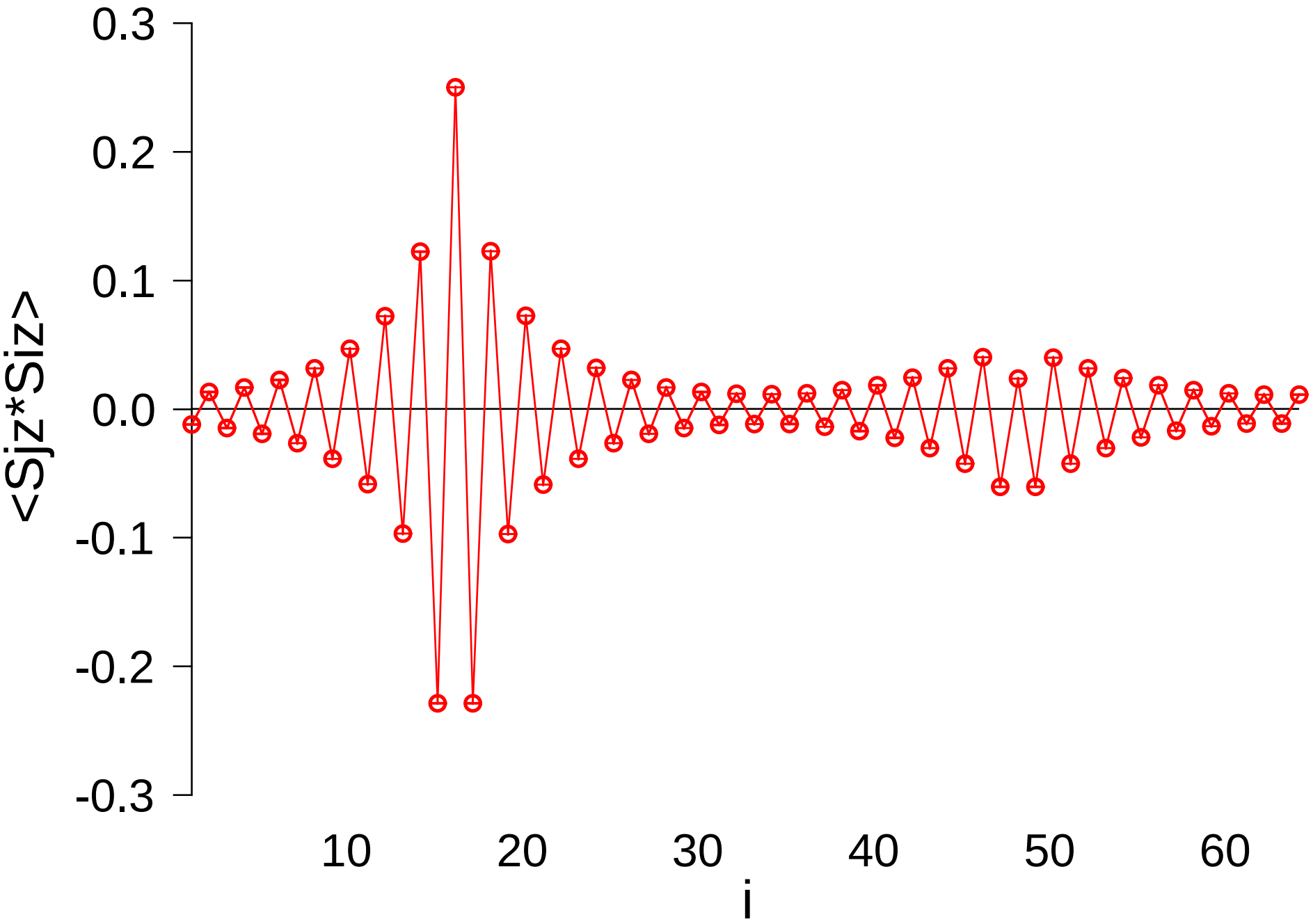

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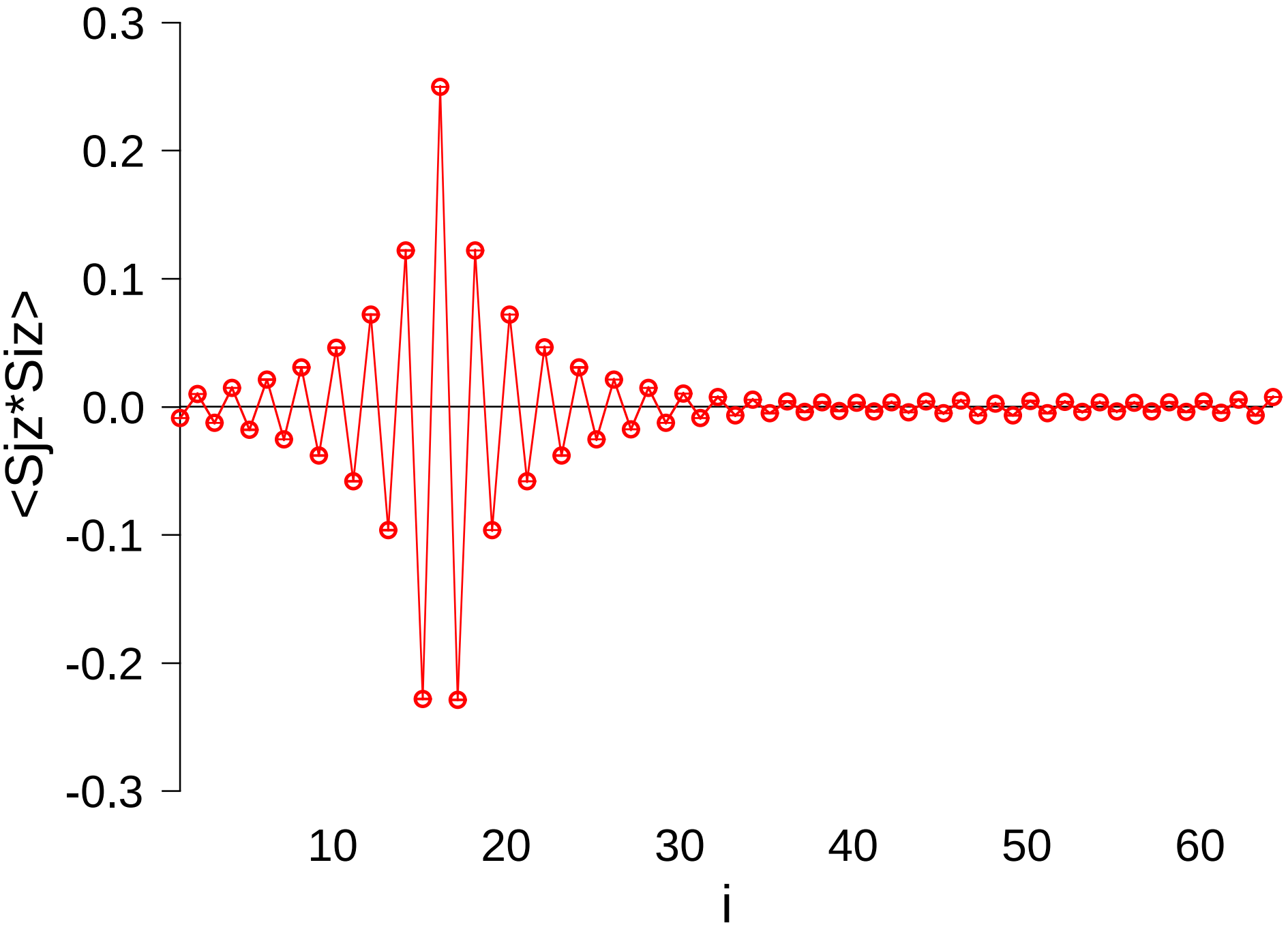

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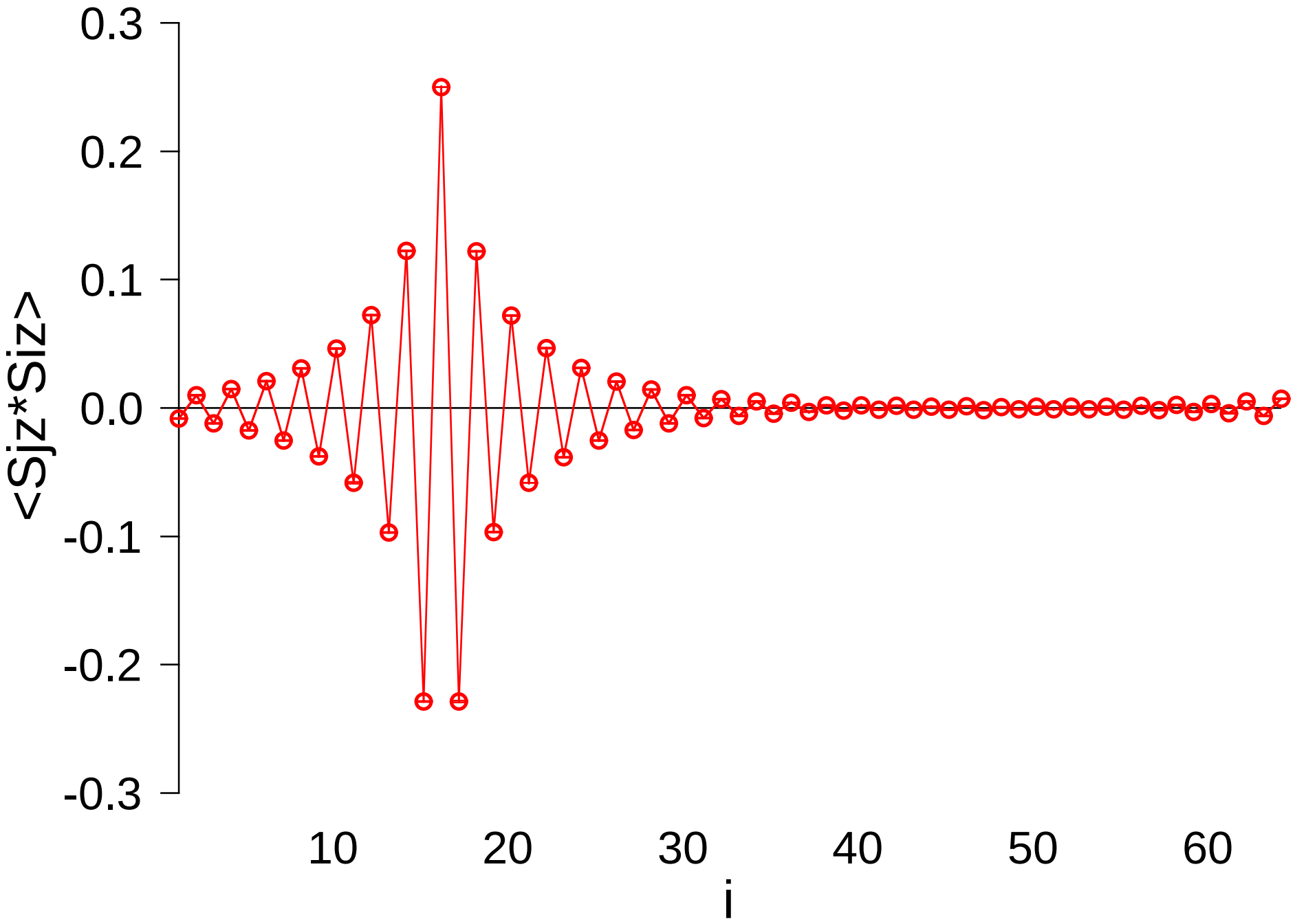

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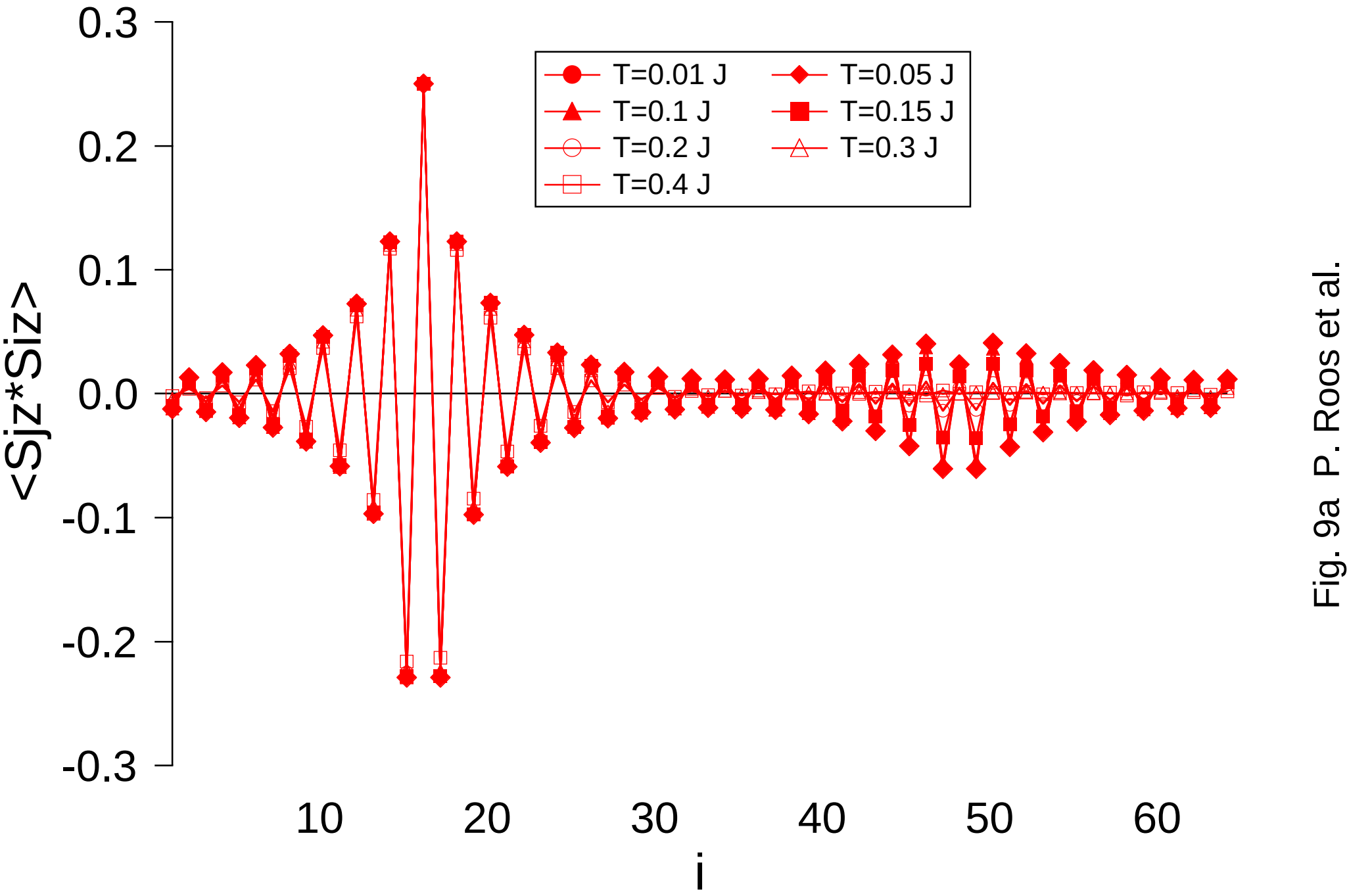

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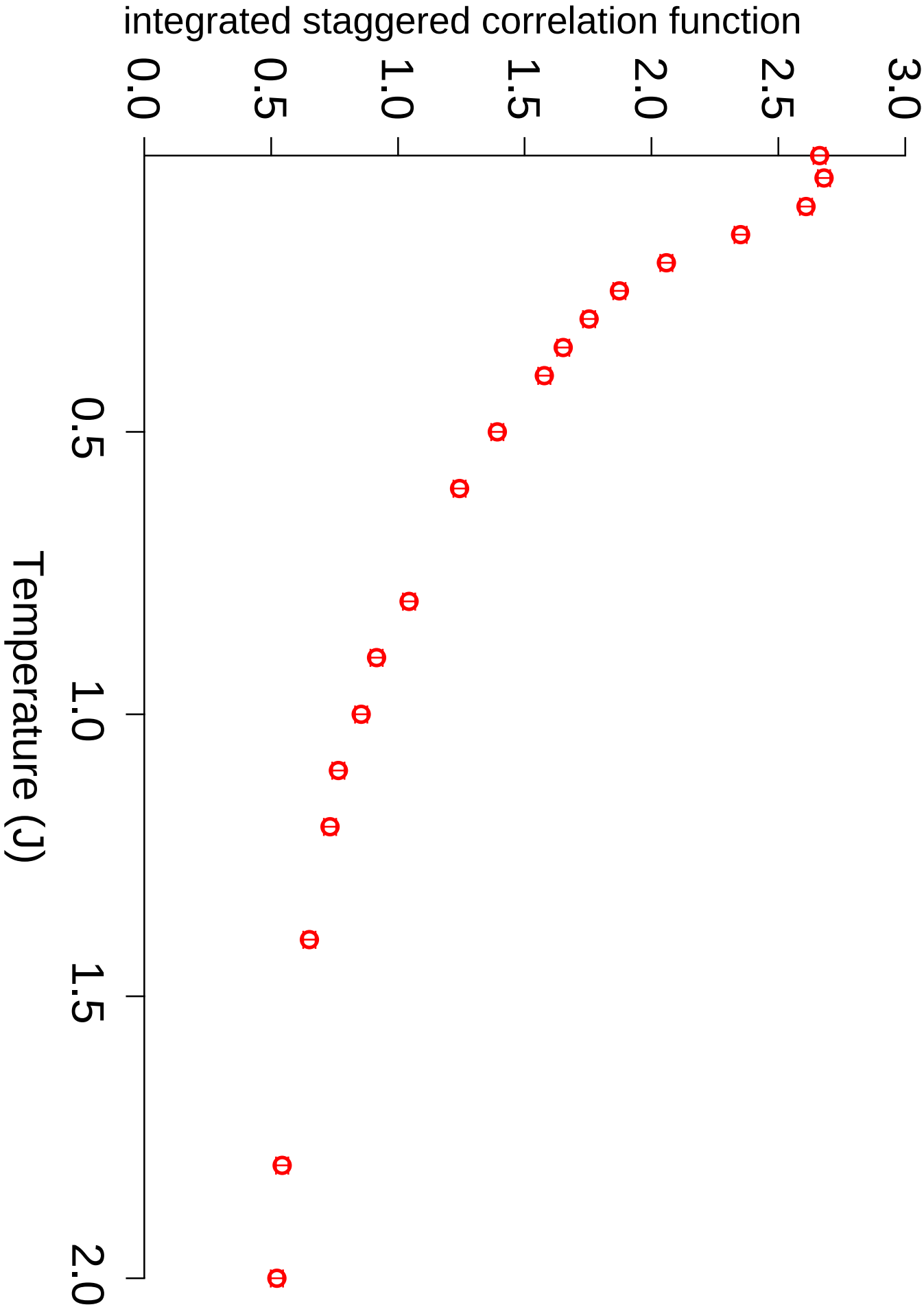

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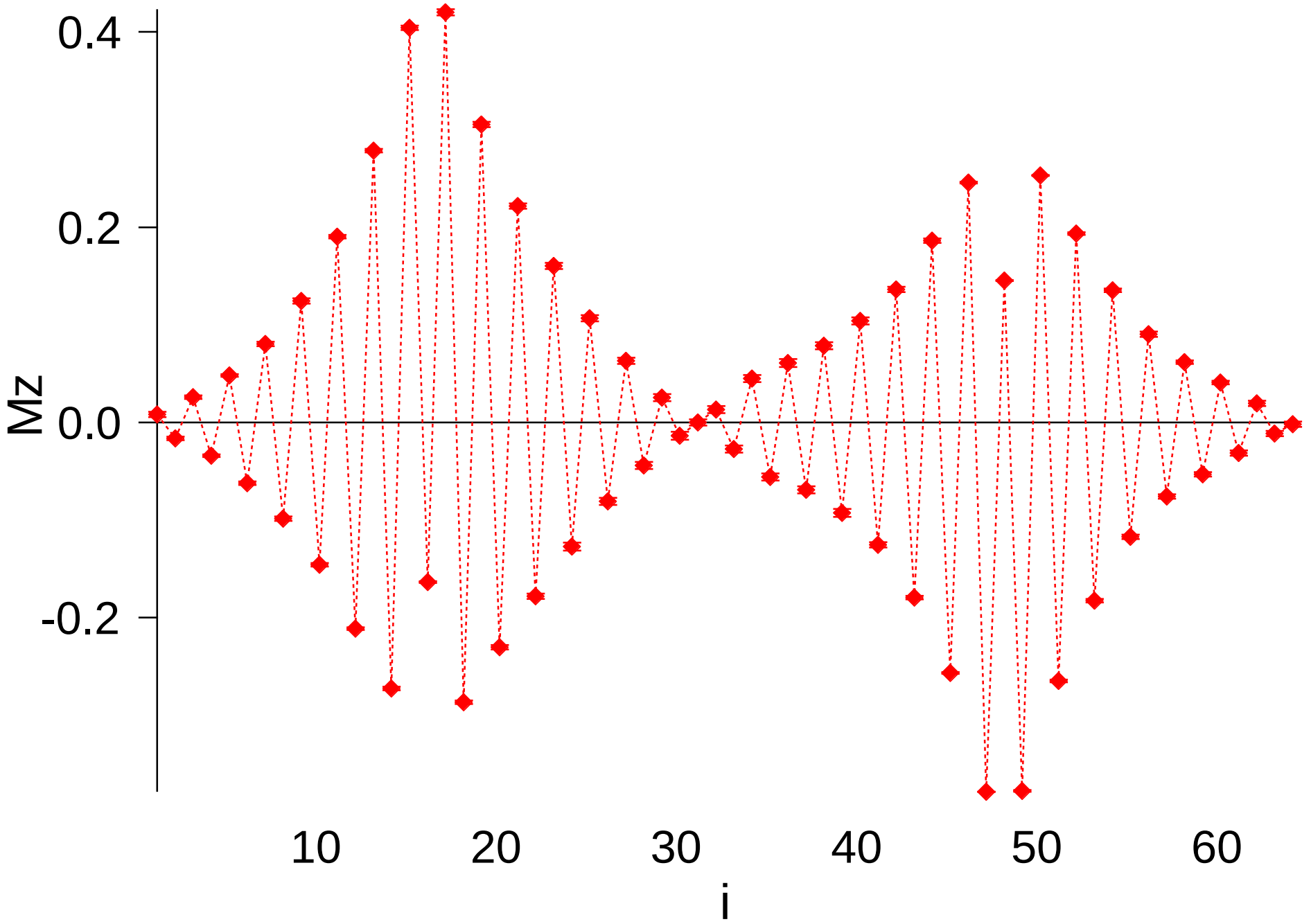

Fig.10 P. Roos et al.

Table	$N_{-1}+N_{-1}$	N_0	$N_{-2}+N_{-2}$	$N_{-3}+N_{-3}$
T=0.2J	48513±58	37724±50	12085±66	1538±14
T=0.15J	49849±60	43930±58	5900±53	322±15
T=0.1J	50616±87	48161±55	1206±15	14±1
T=0.07J	50822±27	49031±59	144±6	14±1
T=0.05J	51437±72	48880±83	9±1	
T=0.03J	51800±57	48199±56		
T=0.01J	55168±81	44830±48		
T=0	$\frac{2}{3}*10^5$	$\frac{1}{3}*10^5$		

Table I P. Roos et al.